

Electrical characteristics of Al contact to NiSi using thin W layer as a barrier

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We show that the thermal instability that is observed in Schottky diodes with an Al film on NiSi contact to (Si) can be removed by introducing a very thin (~ 250 Å) tungsten film between the Al and the NiSi layers. This structure can be formed by sequential evaporation of Ni, W, and Al and subsequent thermal annealing to form NiSi. Schottky barrier measurements show that the contact is thermally stable at 450 °C up to about 1-h annealing with very little change in the electronic barrier height. A model, derived from the electrical measurements, is proposed for the failure mode of the tungsten barrier after excessive annealing.

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Due to the reproducibility of their electrical characteristics, silicides and silicide contacts to Si substrate have received much attention recently as materials to form ohmic contacts, Schottky rectifiers, and interconnections for integrated circuits.^{1,2} Since Al is usually used for final contact to other devices or to bonding pads, the compatibility of Al layer on silicide contact is a problem of practical interest. Previous studies have shown that Ni,³ Pt,⁴ Pd,⁵ Co,⁶ Mo,⁶ and Pt_xNi_{1-x} (Ref. 6) silicides react with Al in the temperature range used for sintering the Al contacts (400–500 °C). Only Ta and Ti silicides were reported as immune to reaction with Al in the above temperature range.

In all other cases, Al reacts with the silicide, leading to the intermetallics of aluminum with the metal from the silicide. Simultaneously, a rise in the SBH (Schottky Barrier Height) is observed causing instability of the contact to the Si substrate and thus making the contact unpractical. In this letter, we consider only *n*-type substrates, and the SBH quoted are therefore the barrier heights for electrons. We investigated the Al-NiSi reaction⁷ and proposed a practical solution to the problem of Al contact to Ni silicide, using a thin W film as diffusion barrier between the Al and the NiSi layers. In this letter, we investigate the electrical characteristic of that Al/W/NiSi/Si contact, compare it to that of the Al/NiSi/Si contact, and we verify that the previously proposed solution is not only structurally, but also electrically stable.

To detect and characterize the films, backscattering spectrometry (BS) was used as an analytical tool. The use of very thin (~ 2 kÅ) underlying Si single-crystal substrate enables us to analyze our samples from the back, through the Si substrate, and thus eliminate the overlap between the Al and Si signals.⁷ The substrates were prepared using a selective etch, following the procedure that was reported elsewhere.⁸

The electrical and structural characteristics of the Al-nickel silicide interaction have been investigated before.^{3,7} It was found that upon heat treatment (285 °C for 4 h or 400 °C for 10 min) the NiSi layer is transformed to the intermetallic NiAl₃. The Si originally present in the NiSi quite probably dissolves in the Al layer. However, the incorporation of thin (~ 250 Å) tungsten barrier under the Al layer inhibits the reaction, and furthermore, there is no need for *in situ* annealing in order to make a reliable contact. Sequential deposition of Ni/W/Al can be followed by annealing outside the depo-

sition chamber. Figure 1 gives the spectra of such a sample as-deposited and after 18- and 64-min anneal at 430 °C. We observe the formation of NiSi, but no Al interaction is observed.

In the present study, we investigate the electrical characteristics of this metallization scheme using forward current-voltage measurements to determine the SBH. For these measurements, a set of samples was prepared on 0.003-Ω cm *n*⁺ substrates with 10-μm-thick 10-Ω cm *epi* layer. After a standard cleaning process of the wafers, the Ni, W, and Al films were sequentially evaporated, without breaking the vacuum, from a 3-source copper hearth using *e*-beam heating. During deposition the powers were approximately 0.8, 0.7, and 1.5 kW, the evaporation rates were approximately 30, 30, and 8 Å/s, and the pressures 4×10^{-7} , 2×10^{-7} , and 10^{-6} Torr for Ni, W, and Al, respectively. The purity of the Ni and W were 99.98% and of the Al, 99.9%. The substrate was thermally coupled to a massive holder and was thereby kept close to room temperature during the deposition. We used a metal mask to define circular areas of 1.6×10^{-2} cm². The film thicknesses were 1.2 kÅ of Ni, 260 Å of W, and 2 kÅ of Al.

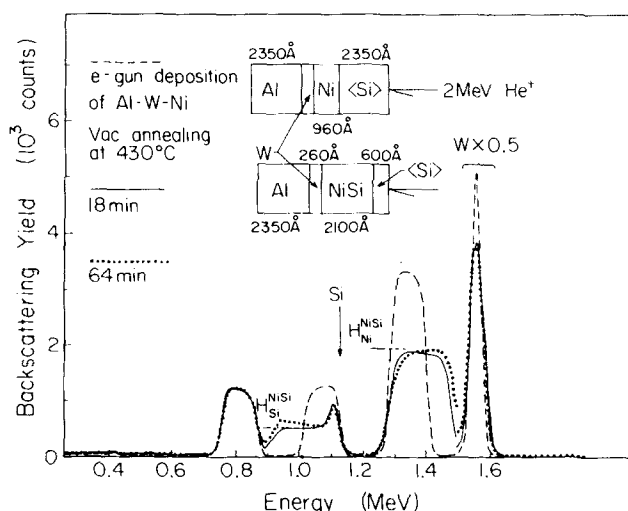


FIG. 1. 2-MeV Backscattering spectra of Al/W/NiSi/(Si) contact. The analyzing beam impinges on the (Si) side. The spectrum of the as-deposited sample (dashed line) clearly depicts the four elemental layers. Annealing at 430 °C transforms the Ni layer to NiSi. The Al signal is unaffected showing that the integrity of the Al layer is preserved.

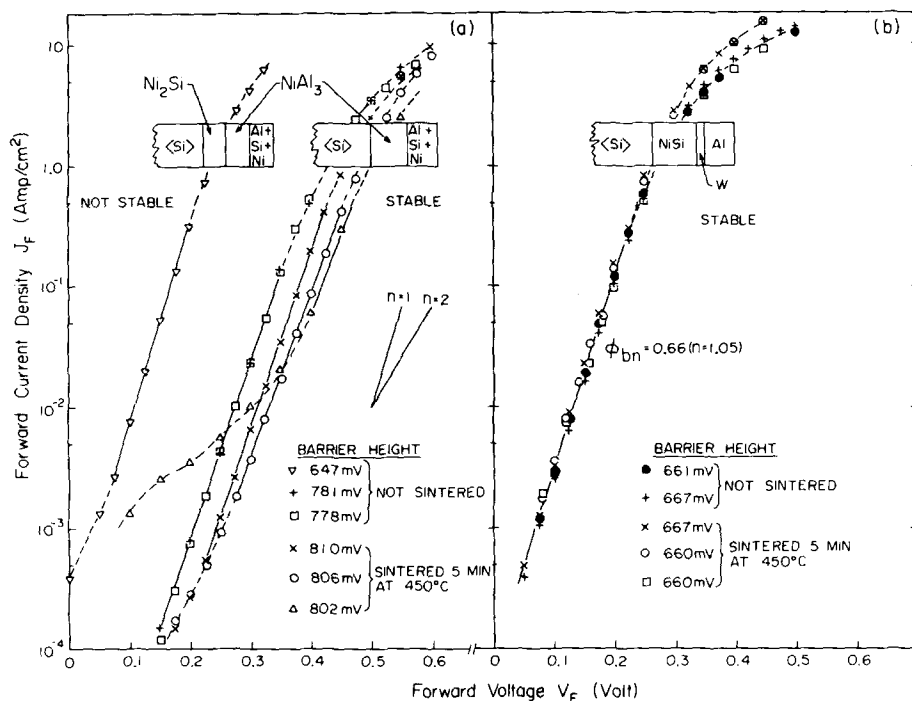


FIG. 2. Forward I - V characteristics used to determine the electron SBH ϕ_{bn} by extrapolation of $\ln J_F$ to zero V_F to determine J_s and using Eq. (1) to find ϕ_{bn} . (a) Al contact on NiSi. The metallization scheme is not stable. Annealing raises the SBH. (b) Al contact on NiSi with a thin W barrier film in between. The diode characteristics do not change during sintering. The SBH is 0.66 V, as reported for NiSi (Ref. 10).

One group of samples was made without W film. Samples were annealed for different times between 5 to 150 min at 450 °C in a N_2 ambient to simulate Al sintering step. The wafers were then scribed and broken, the dies were mounted on TO-5 headers with Au-Si preforms at ~ 400 °C and two 5-mil Al wires were ultrasonically bonded to the front Al contact.

Standard forward dc current-voltage measurements were used to determine the SBH. The thermionic emission model is assumed and the barrier height is deduced from the current density J_s according to

$$\phi_{bn} = (kT/q) \ln(A^{**}T^2/J_s), \quad (1)$$

where A^{**} is the Richardson constant (taken as $110 \text{ A cm}^{-2} \text{ K}^{-2}$ for n -type silicon), T is the absolute temperature, k is Boltzman's constant, and q is the electronic charge. J_s was obtained by linearly extrapolating to zero voltage the logarithm of the forward current density. Since our devices were not passivated and hence have substantial peripheral leakage, this procedure to measure the SBH is the only reliable method available. Figure 2(a) includes a sample (Δ) which is extremely leaky to demonstrate that even in such an extreme case, the leakage current does not prevent a reliable measurement of the SBH because the bulk resistance of the wafers used is low.

Figure 2(a) describes the forward characteristics of samples prepared without W barrier layer. We tried to minimize the heat treatment for some of our samples by not sintering them at all (the only heat treatment was die attaching), but we found only one device (∇) that actually had a barrier height that corresponded to Ni silicide (660 mV).⁹ The other samples all had a SBH within 790 ± 20 mV. This value is in good agreement with a previously reported³ value of 0.76 V from I - V measurements and 0.8 V from C - V measurement for Al-reacted NiSi. Without Al, NiSi contacts to Si are elec-

trically stable under the heat treatments considered in this letter.

The BS analysis of samples without W barrier establishes the existence of an intimate contact of the compound $NiAl_3$ to Si after annealing.⁷ It is thus conceivable that the measured SBH of 800 mV is that of $NiAl_3$ on n -type Si as was previously proposed.³ But another interpretation can be proposed, according to which the rise in the barrier height is due to a very shallow Al-doped Si junction.^{10,11} According to this model, Al that comes into contact with the Si substrate dissolves some Si at the sintering temperature of 450 °C and also the Al and the $NiAl_3$ compound contain the Si atoms previously incorporated in the NiSi layer. During the cooling period, while the wafers are taken out of the annealing furnace, a thin layer of Al-doped Si regrows epitaxially. This thin p -type layer effectively raises the SBH.¹¹

Figure 2(b) describes the characteristics of devices that were made using a thin (250 Å) W barrier. Clearly, the $I(V)$ characteristics are insensitive to heat treatment and all yield the same SBH of 660 ± 10 mV, which is the barrier height of NiSi. Subsequent annealing for 70 min enhances the average barrier height of 10 devices by about 15 mV. This increase is systematic, but falls within uncertainties of an individual measurement. This means in practical applications annealing for about 1 h at 450 °C is an acceptable procedure.

To further test the effectiveness of the W layer in this metallization scheme, the thermal annealing was pursued until the barrier began to fail. We annealed the samples for 2.5 h at 450 °C. Figure 3 describes two typical samples after this long heat cycle. We clearly see an increase from the initial SBH of 660 mV toward the final 800 mV. The measured data can be interpreted as a uniform contact with SBH of 700 ± 20 mV. However, these results can also be modeled in terms of localized failures of the W barrier, a process that is fairly likely for a thin film.

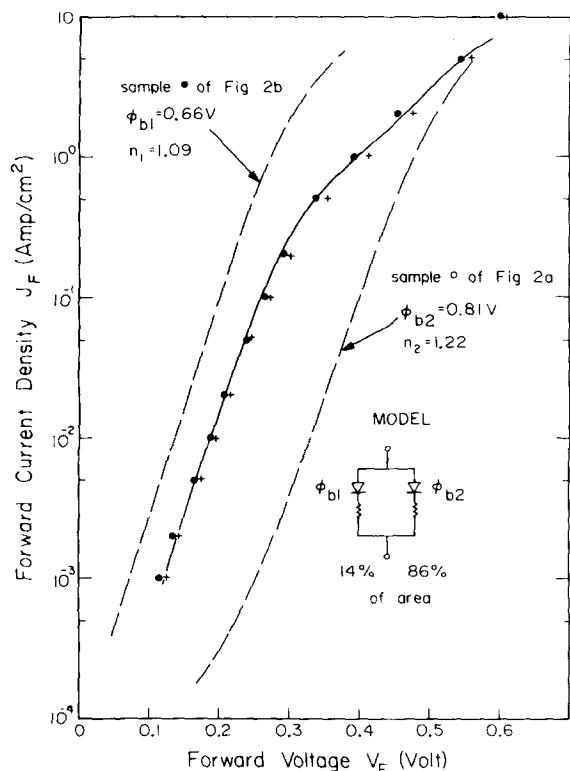


FIG. 3. Forward I - V characteristics of two typical samples (\bullet , $+$) after $2\frac{1}{2}$ -h annealing at 450°C . The outer dashed lines describe the characteristics of the two cases of a reacted and a unreacted NiSi diode, as taken from Fig. 2. The measured characteristics can be interpreted as resulting from two parallel connected diodes (ϕ_{b1} , n_1 , and ϕ_{b2} , n_2) with a relative area of 13.5 and 86.5%, respectively, and $0.75\text{-}\Omega$ total series resistance (solid line).

This model has already been proposed elsewhere in connection with thermally induced changes of Schottky barriers.¹² The model represents the sample in terms of an equivalent circuit with two diodes in parallel. One diode has a low barrier height ($\phi_{bn} \sim 660\text{ mV}$) and the other a high SBH ($\phi_{bn} \sim 800\text{ mV}$), standing for a NiSi contact to Si and Al-reacted NiSi contact to Si. The area ratio between the two diodes will determine the actual I - V characteristics. Since each of the diodes has area that is less than the total device area, the effect of a series resistance is strongest on the low SBH diode. The total series resistance of our devices has been determined from the high current density range of the characteristics and amounts to about $0.7\text{ }\Omega$. The epi layer resistivity by itself contributes $0.625\text{ }\Omega$.

According to that model, the samples presented in Fig. 3 have approximately 14% of their area in the original form of NiSi on Si. The calculated solid line in Fig. 3 was obtained by adjusting the relative areas of the two limiting cases as presented in Fig. 2. Sample \bullet of Fig. 2(b) was modeled as

Schottky diode with $\phi_b = 661\text{ mV}$ and $n = 1.086$. Sample \circ of Fig. 2(a) gives values of 806 mV and 1.22 for the barrier height and ideality factor, respectively. The relative area is 13.5 and 86.5% for the low and high barrier height contact, respectively. The total series resistance in this calculated curve is $0.75\text{ }\Omega$. This interpretation suggests that the W barrier does not fail uniformly. Rather, localized weak spots are permeated by the Al which then reacts with the underlying Ni silicide nonuniformly.

It is worth mentioning that a parallel diode arrangement yields misleading results when its characteristic is interpreted in terms of a laterally uniform contact.¹² The literature of Al contacts to silicide layers on Si contains several reports of unusual SBH and ideality factors.^{4,5,13}

In summary, we have shown that a thin tungsten barrier (250 \AA) is effective in maintaining the integrity of the I - V characteristics of Ni silicide contacted with Al for temperatures up to 450°C for 70 min. We do not explain how that thin W layer functions as a diffusion barrier, but the available evidence suggests that the failure is a localized one if the thermal stressing is excessive. Sintering and encapsulation treatments are well within the acceptable regime of that contacting scheme.

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